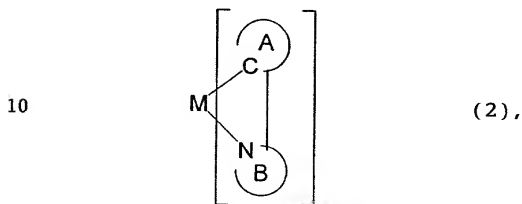


# CLAIMS

1. A metal coordination compound having at least one partial structure represented by formula (1) below:

5 ML (1),

wherein the partial structure ML is represented by formula (2) below:



wherein M is a metal atom of Ir, Pt, Rh or Pd; N and C are nitrogen and carbon atoms, respectively; A is a cyclic group capable of having a substituent, including the carbon atom and bonded to the metal atom M via the carbon atom; B is an isoquinolyl group capable of having a substituent, including the nitrogen atom and bonded to the metal atom M via the nitrogen atom, with the proviso that one or two of CH groups forming the isoquinolyl group can be replaced with a nitrogen atom and the cyclic group A is coordination-bonded to a position-1 carbon atom of the isoquinolyl group;

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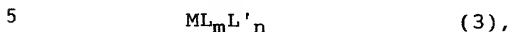
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25 the optional substituent of the cyclic groups is selected from a halogen atom, a cyano group, a nitro group, a di-substituted amino group {of which

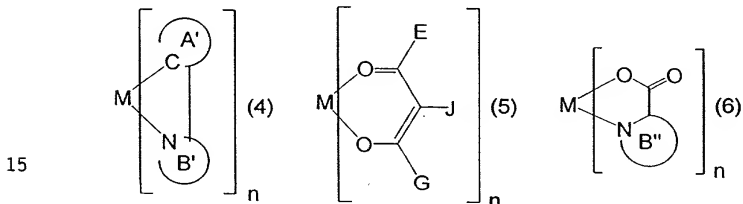
substituents are independently a phenyl group or a naphthyl group each capable of having a substituent (which is selected from a halogen atom, a methyl group or a trifluoromethyl group), or a linear or branched alkyl group having 1 to 8 carbon atoms and including a hydrogen atom optionally replaced with a fluorine atom}, a trialkylsilyl group of which the alkyl groups are independently a linear or branched alkyl group having 1 to 8 carbon atoms, or a linear or branched alkyl group having 1 to 20 carbon atoms {of which the alkyl group can include one or non-neighboring two or more methylene groups that can be replaced with -O-, -S-, -CO-, -CO-O-, -O-CO-, -CH=CH-, -C≡C-, or a divalent aromatic group capable of having a substituent (that is a halogen atom, a cyano atom, a nitro atom, a trialkylsilyl group (of which the alkyl groups are independently a linear or branched alkyl group), a linear or branched alkyl group having 1 to 20 carbon atoms (of which the alkyl group can include one or non-neighboring two or more methylene groups that can be replaced with -O-, -S-, -CO-, -CO-O-, -O-CO-, -CH=CH- or -C≡C-, and the alkyl group can include a hydrogen atom that can be optionally replaced with a fluorine atom)), and the alkyl group can include a hydrogen atom that can be optionally replaced with a fluorine atom}, with the proviso that an adjacent pair of substituents can be bonded to form

a cyclic structure.

2. A metal coordination compound according to Claim 1, represented by formula (3) below:



wherein M is a metal atom of Ir, Pt, Rh or Pd; L and L' are mutually different bidentate ligands; m is 1, 2 or 3 and n is 0, 1 or 2 with the proviso that m+n is 2 or 3; a partial structure  $ML'_n$  is represented by formula (4), (5) or (6) shown below:



wherein N and C are nitrogen and carbon atoms, respectively; A' is a cyclic group capable of having a substituent, including the carbon atom and bonded to the metal atom M via the carbon atom; B' and B'' are each cyclic group capable of having a substituent, including the nitrogen atom and bonded to the metal atom M via the nitrogen atom with the proviso that the cyclic group A' and the cyclic group B' are coordination-bonded to each other;

the optional substituent of the cyclic groups is selected from a halogen atom, cyano group, a nitro

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group, a di-substituted amino group {of which substituents are independently a phenyl group or a naphthyl group each capable of having a substituent (which is selected from a halogen atom, a methyl group  
5 or a trifluoromethyl group), or a linear or branched alkyl group having 1 to 8 carbon atoms and including a hydrogen atom optionally replaced with a fluorine atom}, a trialkylsilyl group of which the alkyl groups are independently a linear or branched alkyl group  
10 having 1 to 8 carbon atoms, or a linear or branched alkyl group having 1 to 20 carbon atoms {of which the alkyl group can include one or non-neighboring two or more methylene groups that can be replaced with -O-, -S-, -CO-, -CO-O-, -O-CO-, -CH=CH-, -C≡C-, or a  
15 divalent aromatic group capable of having a substituent (that is a halogen atom, a cyano atom, a nitro atom, a trialkylsilyl group (of which the alkyl groups are independently a linear or branched alkyl group), a linear or branched alkyl group having 1 to  
20 20 carbon atoms (of which the alkyl group can include one or non-neighboring two or more methylene groups that can be replaced with -O-, -S-, -CO-, -CO-O-, -O-CO-, -CH=CH- or -C≡C-, and the alkyl group can include a hydrogen atom that can be optionally  
25 replaced with a fluorine atom)), and the alkyl group can include a hydrogen atom that can be optionally replaced with a fluorine atom}, with the proviso that

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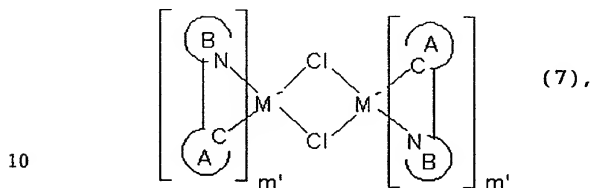
an adjacent pair of substituents can be bonded to form a cyclic structure; and

E, G and J are independently a linear or branched alkyl group having 1 to 20 carbon atoms {of which the alkyl group can include one or non-  
5 neighboring two or more methylene groups that can be replaced with -O-, -S-, -CO-, -CO-O-, -O-CO-, -CH=CH-, -C≡C-, or a divalent aromatic group capable of having a substituent (that is a halogen atom, a cyano atom, a  
10 nitro atom, a trialkylsilyl group (of which the alkyl groups are independently a linear or branched alkyl group), a linear or branched alkyl group having 1 to 20 carbon atoms (of which the alkyl group can include one or non-neighboring two or more methylene groups  
15 that can be replaced with -O-, -S-, -CO-, -CO-O-, -O-CO-, -CH=CH- or -C≡C-, and the alkyl group can include a hydrogen atom that can be optionally replaced with a fluorine atom) with the proviso that an adjacent pair of substituents can be bonded to form  
20 a cyclic structure), and the alkyl group can include a hydrogen atom that can be optionally replaced with a fluorine atom}, or di-substituted amino group {of which substituents are independently a phenyl group or a naphthyl group each capable of having a substituent  
25 (which is selected from a halogen atom, a methyl group or a trifluoromethyl group), or a linear or branched alkyl group having 1 to 8 carbon atoms and including a

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hydrogen atom optionally replaced with a fluorine atom}, and J can also be a hydrogen atom.

3. A metal coordination compound according to  
5 Claim 1, represented by formula (7) below:



wherein Cl denotes a chlorine atom, M' denotes iridium Ir or rhodium Rh, and m' is 2.

- 15 4. A metal coordination compound according to  
Claim 2, including a partial structure  $ML'_n$   
represented by the formula (4) in the formula (3).

- 20 5. A metal coordination compound according to  
Claim 2, including a partial structure  $ML'_n$   
represented by the formula (5) in the formula (3).

- 25 6. A metal coordination compound according to  
Claim 2, including a partial structure  $ML'_n$   
represented by the formula (6) in the formula (3).

7. A metal coordination compound according to

Claim 2, wherein n is 0 in the formula (3).

8. A metal coordination compound according to Claim 2, wherein the cyclic groups A and A' are  
5 independently selected from phenyl group, naphthyl group, thienyl group, fluorenyl group, thianaphthyl group, acenaphthyl group, anthranyl group, phenanthrenyl group, pyrenyl group, or carbazolyl group, as an aromatic cyclic group capable of having a  
10 substituent with the proviso that the aromatic cyclic group can include one or two CH groups that can be replaced with a nitrogen atom.

9. A metal coordination compound according to  
15 Claim 8, wherein the cyclic groups A and A' are selected from phenyl group, 2-naphthyl group, 2-thienyl group, 2-fluorenyl group 2-thianaphthyl group, 2-anthranyl group, 2-phenanthrenyl group, 2-pyrenyl group, or 3-carbazolyl group, as an aromatic cyclic  
20 group capable of having a substituent with the proviso that the aromatic cyclic group can include one or two CH groups that can be replaced with a nitrogen atom.

10. A metal coordination compound according to  
25 Claim 9, wherein the aromatic cyclic group is phenyl group capable of having a substituent.

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11. A metal coordination compound according to  
Claim 10, wherein a hydrogen atom is attached to a  
position-6 carbon atom of the phenyl group capable of  
having a substituent next to a position-1 carbon atom  
5 bonded to the cyclic group B.

12. A metal coordination compound according to  
Claim 2, wherein the cyclic groups B' and B" are  
independently selected from isoquinolyl group,  
10 quinolyl group, 2-azaanthranyl group, phenanthridinyl  
group, pyridyl group, oxazolyl group, thiazolyl group,  
benzoxazolyl group, or benzthiazolyl group, as an  
aromatic cyclic group capable of having a substituent  
with the proviso that the aromatic cyclic group can  
15 include one or two CH groups that can be replaced with  
a nitrogen atom.

13. A metal coordination compound according to  
Claim 12, wherein the cyclic groups B' and B" are  
20 selected from isoquinolyl group or pyridyl group, as  
an aromatic cyclic group capable of having a  
substituent with the proviso that the aromatic cyclic  
group can include one or two CH groups that can be  
replaced with a nitrogen atom.

25

14. A metal coordination compound according to  
Claim 2, wherein the cyclic group B' in the formula



(4) is isoquinolyl group capable of having a substituent.

15. A metal coordination compound according to  
5 Claim 2, wherein the cyclic groups A, A', B, B' and B" are independently non-substituted, or have a substituent selected from a halogen atom or a linear or branched alkyl group having 1 to 20 carbon atoms {of which the alkyl group can include one or non-  
10 neighboring two or more methylene groups that can be replaced with -O-, -S-, -CO-, -CO-O-, -O-CO-, -CH=CH-, -C≡C-, or a divalent aromatic group capable of having a substituent (that is a halogen atom, or a linear or branched alkyl group having 1 to 20 carbon atoms (of  
15 which the alkyl group can include one or non-neighboring two or more methylene groups that can be replaced with -O-, and the alkyl group can include a hydrogen atom that can be optionally replaced with a fluorine atom)), and the alkyl group can include a  
20 hydrogen atom that can be optionally replaced with a fluorine atom}.

16. A metal coordination compound according to  
Claim 3, wherein the cyclic group A in the formula (7)  
25 is selected from phenyl group, naphthyl group, thienyl group, fluorenyl group, thianaphthyl group, acenaphthyl group, anthranyl group, phenanthrenyl

group, pyrenyl group, or carbazolyl group, as an aromatic cyclic group capable of having a substituent with the proviso that the aromatic cyclic group can include one or two CH groups that can be replaced with a nitrogen atom.

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17. A metal coordination compound according to Claim 16, wherein the aromatic cyclic group is selected from phenyl group, 2-naphthyl group, 2-thienyl group, 2-fluorenyl group, 2-thianaphthyl group, 2-anthranyl group, 2-phenanthrenyl group, 2-pyrenyl group or 3-carbazolyl group, each capable of having a substituent with the proviso that the aromatic cyclic group can include one or two CH groups that can be replaced with a nitrogen atom.

18. A metal coordination compound according to Claim 17, wherein the aromatic cyclic group is phenyl group capable of having a substituent.

19. A metal coordination compound according to Claim 18, wherein a hydrogen atom is attached to a position-6 carbon atom of the phenyl group capable of having a substituent next to a position-1 carbon atom bonded to the cyclic group B.

20. A metal coordination compound according to

Claim 3, wherein the cyclic groups A and B in the formula (7) are independently non-substituted, or have a substituent selected from a halogen atom or a linear or branched alkyl group having 1 to 20 carbon atoms  
5 {of which the alkyl group can include one or non-neighboring two or more methylene groups that can be replaced with -O-, -S-, -CO-, -CO-O-, -O-CO-, -CH=CH-, -C=C-, or a divalent aromatic group capable of having a substituent (that is a halogen atom, a cyano atom, a  
10 nitro atom, a trialkylsilyl group (of which the alkyl groups are independently a linear or branched alkyl group), a linear or branched alkyl group having 1 to 20 carbon atoms (of which the alkyl group can include one or non-neighboring two or more methylene groups  
15 that can be replaced with -O-, and the alkyl group can include a hydrogen atom that can be optionally replaced with a fluorine atom)), and the alkyl group can include a hydrogen atom that can be optionally replaced with a fluorine atom}.

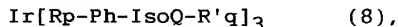
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21. A metal coordination compound according to Claim 1, wherein M in the formula (1) is iridium.

22. A metal coordination compound according to  
25 Claim 3, wherein M in the formula (7) is iridium.

23. A metal coordination compound according to

Claim 1 or 2, having a partial structure ML  
represented by the formula (2) and represented by  
formula (8) below:



- 5 wherein Ir is iridium; partial structure Ph-IsoQ  
denotes 1-phenylisoquinolyl group; substituents R and  
R' are selected from hydrogen, fluorine or a linear or  
branched alkyl group represented by  $\text{C}_n\text{H}_{2n+1}$  (wherein H  
can be replaced with F, a non-adjacent methylene group  
10 can be replaced with oxygen and n is an integer of 1  
to 20), p and q are integers of at least 1  
representing numbers of the substituents R and R'  
bonded to the phenyl group and the isoquinolyl group,  
respectively, wherein a position-2 carbon atom of the  
15 phenyl group and a nitrogen atom of IsoQ are  
coordination-bonded to Ir.

24. A metal coordination compound according to  
Claim 23, wherein the partial structure Rp-Ph is 4-  
20 alkylphenyl group in the formula (8), and the  
substituent R' is hydrogen.

25. A metal coordination compound according to  
Claim 23, wherein in the formula (8), the substituent  
25 R is hydrogen, and R'q represents a fluoro or  
trifluoromethyl group substituted at a 4- or 5-  
position.

26. A metal coordination compound according to  
Claim 23, wherein in the formula (8), the partial  
structure Rp-Ph- is 5-fluorophenyl group, and R'q is a  
5 hydrogen atom or a fluorine atom or trifluoromethyl  
group substituted at a 4- or 5-position.

27. A metal coordination compound according to  
Claim 23, wherein in the formula (8), the partial  
10 structure Rp-Ph- is 4-fluorophenyl group, and R'q is a  
hydrogen atom or a fluorine atom or trifluoromethyl  
group substituted at a 4- or 5-position.

28. A metal coordination compound according to  
15 Claim 23, wherein in the formula (8), the partial  
structure Rp-Ph- is 3,5-difluorophenyl group, and R'q  
is a hydrogen atom or a fluorine atom or trifluoro-  
methyl group substituted at a 4- or 5-position.

29. A metal coordination compound according to  
20 Claim 23, wherein in the formula (8), the partial  
structure Rp-Ph- is 3,4,5-trifluorophenyl group, and  
R'q is a hydrogen atom or a fluorine atom or  
trifluoromethyl group substituted at a 4- or 5-  
25 position.

30. A metal coordination compound according to

Claim 23, wherein in the formula (8), the partial structure Rp-Ph- is 4-trifluoromethylphenyl group, and R'q is a hydrogen atom or a fluorine atom or trifluoromethyl group substituted at a 4- or 5- position.

31. A metal coordination compound according to Claim 23, wherein in the formula (8), the partial structure Rp-Ph- is 5-trifluoromethylphenyl group, and R'q is a hydrogen atom or a fluorine atom or trifluoromethyl group substituted at a 4- or 5- position.

32. A metal coordination compound according to Claim 23, wherein in the formula (8), the structure Rp-Ph is a 1-(3,4,5,6-tetrafluoromethyl)phenyl group, and in R'q, q is 1 or 6 and R' is a hydrogen atom or a trifluoromethyl group or 3,4,5,6,7,8-hexafluoro group substituted at a 4- or 5-position.

33. A metal coordination compound according to Claim 23, wherein in the formula (8), the partial structure Rp-Ph- is 4-alkylphenyl group (wherein the alkyl group is a linear or branched alkyl group having 1 to 6 carbon atoms), and R'q is hydrogen.

34. A metal coordination compound according to

Claim 23, wherein in the formula (8), the partial structure  $R_p\text{-Ph-}$  is 4-alkoxyphenyl group (wherein the alkoxy group is a linear or branched alkoxy group having 1 to 6 carbon atoms), and  $R'_q$  is hydrogen.

5

35. A metal coordination compound according to Claim 23, wherein in the formula (8), the partial structure  $R_p\text{-Ph-}$  is 4-trifluorooxyphenyl group, and  $R'_q$  is a hydrogen atom or a fluorine atom or trifluoromethyl group substituted at a 4- or 5-position.

36. A metal coordination compound according to Claim 2, which is represented by the formula (3) and is also represented by formula (9) below:



wherein Ir represents iridium.

37. A metal coordination compound according to Claim 36, represented by the formula (9), wherein  $L_m$  is represented by a formula of [4-alkylphenyl-isoquinoline]<sub>2</sub> (wherein the alkyl group is represented by  $C_nH_{2n+1}$  and n is an integer of 1 to 8), and  $L'_n$  is 1-phenylisoquinoline.

25

38. A metal coordination compound according to Claim 36, represented by the formula (9), wherein  $L_m$

is represented by a formula [1-phenylisoquinoline]<sub>2</sub>,  
and L'<sub>n</sub> is 4-alkylphenylisoquinoline (wherein the  
alkyl group has 1 to 8 carbon atoms).

5           39. A metal coordination compound according to  
Claim 1, wherein one or two CH groups in the  
isoquinolyl group capable of having a substituent in  
the formula (1) are replaced with a nitrogen atom.

10           40. A metal coordination compound according to  
Claim 3, wherein one or two CH groups in the  
isoquinolyl group capable of having a substituent in  
the formula (7) are replaced with a nitrogen atom.

15           41. An organic luminescence device, comprising: a  
pair of electrodes disposed on a substrate, and a  
luminescence unit comprising at least one organic  
compound disposed between the electrodes, wherein the  
organic compound comprises a metal coordination  
20           compound having at least one partial structure  
represented by the formula (1) in Claim 1.

            42. An organic luminescence device according to  
Claim 41, wherein the organic compound comprises a  
25           metal coordination compound having a structure  
represented by the formula (3).



43. An organic luminescence device according to Claim 41, wherein the organic compound comprises a metal coordination compound having a structure represented by the formula (8).

5

44. An organic luminescence device according to Claim 41, wherein the organic compound comprises a metal coordination compound having a structure represented by the formula (9).

10

45. An organic luminescence device according to Claim 41, wherein a voltage is applied between the electrodes to emit phosphorescence.

15

46. An organic luminescence device according to Claim 45, wherein the phosphorescence is red in luminescence color.

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47. A picture display apparatus, comprising an organic luminescence device according to any of Claims 41 to 46, and a means for supplying electric signals to the organic luminescence device.

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